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# Recovery of Transport Coefficients in Navier–Stokes Equations from Modeled Boltzmann Equation

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## Introduction

THE objective of this Letter is to show that the full set of compressible Navier–Stokes (NS) equations (which consist of the continuity, the momentum, the thermal energy, and the gas equation of state) can be derived from the modeled Boltzmann equation (BE) [1] by suitably modifying the collision relaxation time $\tau$ in the commonly assumed Bhatnagar, Gross, and Krook (BGK) model [2]. The modeled BE thus derived is valid for dense gas only when the mean free path between two successive particle collisions is very small compared with the characteristic spatial scale of the fluid system $L$. It is not sufficient to show that the NS equations are recovered [3–5]; more important, it has to demonstrate that the transport coefficients (such as bulk viscosity $\mu$, thermal conductivity $\kappa$, and the specific heat ratio $\gamma$) of the fluid can be correctly replicated, because in the solution of the NS equations, these coefficients are specified, but they are part of the solution of the modeled BE.

## Inadequacy of Existing $\tau$ Model

A frequently assumed $\tau$ model is the rigid-sphere model [6]; this results in a single relaxation time $\tau = \tau_1 \approx (5/4)(\bar{\lambda}/|\boldsymbol{\xi}|) \propto (T)^{-1/2}$, where $T$ is the gas temperature, $\bar{\lambda}$ is the average mean free path, and $|\boldsymbol{\xi}| \propto \sqrt{T}$ is the magnitude of the mean particle velocity. The functional dependence of $\tau$ on $(T)^{-1/2}$ is a result of its dependence $|\boldsymbol{\xi}|$. This treatment is tantamount to considering only the translational degree of freedom in particle collisions. The $\tau$ model gives rise to $\mu \propto \tau$ and $\kappa \propto \tau$ and $\gamma = (D+2)/D$, where $D$ is a dimension number. This means that $\gamma$ is only correct for three-dimensional flow ($D = 3$) of monoatomic gases. Therefore, $\gamma$ is not correct for diatomic gases (such as air) and it follows that the calculated Mach number $M = U/c$ (where $U$ is the fluid velocity) is also in error, because $c \propto \gamma^{1/2}$. Because $\tau \propto (T)^{-1/2}$ and the derived $\mu = \rho RT\tau$, the dependence of $\mu$ on $T$ is not consistent with the Sutherland law [6]. Here, $\rho$ is fluid density and $R$ is the universal gas constant. The derived expression for $\kappa$ is $\kappa = c_p\mu$; this leads to an incorrect $\kappa$ dependence on $T$ and a Prandtl number $Pr = c_p\mu/\kappa = 1$, where $c_p$ is the specific heat at constant pressure of the fluid. In other words, the Reynolds number $Re = \rho UL/\mu$; the Mach and Prandtl numbers thus deduced are different from the specifications for the solution of the NS equations [7–11]. An attempt to address this deficiency has been made by postulating a relaxation time matrix $\boldsymbol{S}$ to replace $\tau$ and to solve the modeled BE using the lattice approach [7]. However, the elements of $\boldsymbol{S}$, except $\tau_1$, were not derived from physical consideration, but rather empirically.

Because the Reynolds, Mach, and Prandtl numbers are part of the solution of the modeled BE, their accuracies are important to a correct recovery of the solution of the NS equations from the modeled BE. This is especially true for aeroacoustic and shock-free compressible flow simulations. The present Letter proposes to recover $\mu$ (Reynolds number), $\gamma$ (Mach number), and $\kappa$ (Prandtl number) by adopting a multiple-relaxation-time approach [7], but with the relaxation times derived from physical consideration. This approach does not require solving the modeled BE by the lattice method. The modeled BE can be solved by any numerical scheme and the solution of the NS equations is recovered. An attempt to replicate $\mu$ and $\gamma$ has been made previously [12]. This Letter presents the derivation of $\kappa$. However, for the sake of completeness, a brief description of the derivation of $\mu$ and $\gamma$ is first presented in the next section.

## Recovery of $\mu$ and $\gamma$

From the preceding discussion, it is obvious that if the Reynolds and Mach numbers were to be recovered correctly, the correct $\mu$ dependence on $T$ has to be obtained and $\gamma = 1.4$ has to be replicated for diatomic gases irrespective of the flow dimension number. The phenomenon of fluid viscosity could be attributed to momentum transfer between gas particles before and after collisions. The distributions of momenta of the particles depend on the momentum of each particle when they are widely separated, as well as the interactions of intermolecular potentials when two particles are in close encounter. The intermolecular potential represents the contributions of intermolecular attraction and repulsion to the potential function. According to Ferziger and Kaper [6], a rigid-sphere model poorly predicts the temperature dependence of the macroscopic fluid properties. This is due to an overestimation of the

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potential change over the particle separation $r_m \approx \sigma_m$. Sutherland (see Ferziger and Kaper) suggests to include a weak, but rapidly decaying, repulsive potential, $\sim(\sigma_m/r_m)^n$ ($n$ being the index of repulsion), in the interaction and successfully provides a more realistic description of the dependence of $\mu$ on $T$. The effects of this weak potential might be more pronounced in the relaxation of a diatomic gas, due to its more complicated molecular structure.

An attempt to account for the weak potential is made by including the relaxation times associated with both the intermolecular potential and the weak repulsive potential in the estimate of $\tau$. Therefore, it is suggested to account for the translational and rotational degree of freedom, $D_T$ and $D_R$, in the derivation of an effective relaxation time $\tau_{\text{eff}}$ to replace $\tau$. This $\tau_{\text{eff}}$ was assumed to be made up of two relaxation times, $\tau_1$ and $\tau_2$; $\tau_1$ is representative of the translational relaxation and is given by the rigid-sphere model, whereas $\tau_2$ is chosen to represent the rotational relaxation and could be determined by stipulating a constraint specified by imposing the Sutherland law for $\mu$. Thus formulated, $\mu$ is given by

$$\mu = \rho RT\tau_{\text{eff}} = \frac{\rho RT\tau_1}{(1+\tau_1/\tau_2)} \propto \frac{\sqrt{T}}{(1+\tau_1/\tau_2)} \tag{1}$$

where $R$ is the universal gas constant and $\tau_{\text{eff}} = \tau_1/(1+\tau_1/\tau_2)$. In deriving Eq. (1), the assumption has been made that $\tau_1$ is given by the rigid-sphere model and its dependence on $T$ is therefore given by $\tau_1 \propto (T)^{-1/2}$. The constraint imposed by the Sutherland law then leads to $\tau_1/\tau_2 = S_o/T$, where $S_o$ is the Sutherland constant and an exact determination of $\tau_2$. In other words, $\mu$ as given in Eq. (1) is modified by the factor $1/(1+S_o/T)$ compared with the expression derived assuming the relaxation time to be given by $\tau_1 = \tau$. Once $\mu$ is calculated correctly, the determination of the Reynolds number is also correct. In this two-relaxation-time approach, the ratio of the specific heats is given by $\gamma = (D_T + D_R + 2)/(D_T + D_R)$, which yields $\gamma = 1.4$ for diatomic gases. This implies that the speed of sound, as well as the Mach number, of the aeroacoustic problem can be correctly resolved. However, $\kappa = c_p\mu$ is obtained, implying that $Pr = 1$. This means that the thermal energy exchange between particles has not been replicated properly and the modified BGK model needs further improvement to account for the thermal energy exchange during the collision process.

## Recovery of $\kappa$

In an attempt to further rectify $\kappa$, a modification based on Eucken's theory of heat conduction [13,14] is proposed. The use of Eucken's theory to recover the Fourier law of heat conduction has been attempted before [15,16] and good results were obtained. Eucken suggested splitting the thermal conductivity of a dense gas into two noninteracting parts; one is due to the transport of translational energy and the other is due to the transport of internal energy. Because only the contribution of the rotational degree of freedom to the internal energy transport is considered in the present study, the specific energy $e'$ of a diatomic gas might be expressed as $e' = e'_{\text{tran}} + e'_{\text{rot}} = c'_V T + c''_V T$, where the specific heats at constant volume are given by $c'_V = 3R/2$ and $c''_V = RD_R/2$, respectively [14]. In general, the local heat flux $\boldsymbol{q}$ of a gas can be expressed as $\boldsymbol{q} = \boldsymbol{q}_{\text{unc}} + \boldsymbol{q}_{\text{int}}$, where $\boldsymbol{q}_{\text{unc}} = \rho \boldsymbol{u}u^2/2$ is the uncollided heat flux and $\boldsymbol{q}_{\text{int}} = \rho \boldsymbol{u}e$ is the heat flux due to particle interaction. Starting from Eucken's theory of heat conduction [13,14], it can be shown that the heat flux $\boldsymbol{q}$ is related to the local temperature gradient $\nabla T$, as follows:

$$\boldsymbol{q} = \boldsymbol{q}_{\text{unc}} + \boldsymbol{q}_{\text{int}} = -[\tfrac{5}{2}c'_V p\tau_{\text{eff}} + c''_V p\tau_{\text{eff}}(1+\zeta)]\nabla T \tag{2}$$

where $\zeta$ is a correction factor for thermal relaxation [14]. Using the Fourier law of heat conduction, together with expressions for gas physical properties obtained from the modified BE [6], Eq. (2) could be shown to lead to an expression for $\kappa$, as follows:

$$\kappa = \left|\frac{\vec{q}}{\nabla T}\right| = \frac{5}{2}c'_V p\tau_{\text{eff}} + c''_V p\tau_{\text{eff}}(1+\zeta) = \frac{\mu c_V}{4}(9\gamma + 10\zeta - 6\gamma\zeta - 5) = \frac{c_p\mu}{4\gamma}(9\gamma + 10\zeta - 6\gamma\zeta - 5) \tag{3}$$

Eucken suggested that the ratio $f_E = \kappa/c_V\mu$ between $\kappa$, $c_V$, and $\mu$ should be constant for a specific gas. This ratio is known as Eucken's factor. For diatomic gases, its value is given by $f_E = (9\gamma - 5)/4 + \zeta(5 - 3\gamma)/2$. For air, $\gamma = 1.4$ and $\zeta = 0.15$; this gives rise to $f_E \approx 1.96$, in agreement with the value obtained experimentally [13]. Consequently, the Prandtl number can be expressed in terms of $f_E$, as follows:

$$Pr = \frac{\mu c_p}{\kappa} = \frac{\mu\gamma c_V}{\kappa} = \frac{\gamma}{f_E} \tag{4}$$

According to Eq. (4) and using $f_E \approx 1.96$, $Pr \approx 0.71$, thus showing that the Prandtl number is recovered using this approach to evaluate heat conduction between particles. From Eq. (3), it can be seen that the derived expression for $\kappa$ is modified by the factor $(9\gamma + 10\zeta - 6\gamma\zeta - 5)/4\gamma$ compared with the uncorrected case, and this factor is only dependent on $\gamma$ and a correction factor $\zeta$ for thermal relaxation. It should be noted that the expression for the thermal diffusivity $\kappa'$ is given by $\kappa' = f_E\mu = \kappa/c_V = f_E(\gamma - 1)\rho e\tau_{\text{eff}}$. The net result again is a correction factor given by $f_E/\gamma$. Therefore, this approach to model heat conduction does not require the introduction of another relaxation time to account for thermal energy exchange during the particle collision process.

## Discussion

It can be seen that the introduction of $\tau_1$ and $\tau_2$ is sufficient to account for translational, rotational, and thermal energy exchanges during the particle collision process, and this gives rise to a correct calculation of $\gamma$ and the transport coefficients $\mu$ and $\kappa$ (i.e., the Reynolds, Mach, and Prandtl numbers can be determined correctly in the process of solving the modeled BE). The specific heat ratio $\gamma$ is replicated exactly by taking into account the weak repulsive potential in the collision process. This, together with Sutherland's law, leads to a relation between $\tau_1$ and $\tau_2$ and to the result $\tau_{\text{eff}} = \tau_1/(1+S_o/T)$. The factor $1/(1+S_o/T)$ can be interpreted as a correction factor for $\tau_1$. This correction factor allows $\mu$ (Reynolds number) to be recovered; whereas another correction factor given by $(9\gamma + 10\zeta - 6\gamma\zeta - 5)/4\gamma$ permits $\kappa$ (Prandtl number) to be replicated exactly. Physically, this means that the exchange of linear and angular momentum, and the exchange of thermal energy, occur in the same time scale $\tau_1$; the net exchange results only differ by a correction factor. Furthermore, these results imply that the correct calculation of $\gamma$ is crucial to the recovery of the NS equations and their transport coefficients. This interpretation is drawn because of the interrelation between $\gamma$ and $T$ and the fact that $T$ can be expressed as $c^2/\gamma R$.

The successful recovery of the Reynolds and Mach numbers has been validated by Li et al. [12,17] In their approach, a lattice Boltzmann method was used to solve the modeled BE using a D2Q13 velocity lattice. Aeroacoustic problems were used to carry out the validation and these include the propagation of plane and circular pressure pulse, interaction of acoustic, entropy and vortex pulses, plane sinusoidal wave propagation in a quiescent fluid, and a Gaussian sound pulse. Together, these cases test the ability of the model in their prediction of the propagation speed of sound, the isotropic behavior of sound propagation, and the accuracy of the model. The D2Q13 velocity lattice was sufficient to replicate the aerodynamic and acoustic properties, and they show excellent agreement with either theoretical solutions or with direct numerical simulation results obtained with a sixth-order finite difference scheme, similar to that proposed by Lele [18]. In particular, the Mach number was replicated exactly over a range, $0.01 \le M \le 0.9$. Some of the cases treated by Li et al. were also reported by Tsutahara et al. [9] and Kang et al. , in which a velocity lattice of D2Q21 was assumed. However, their results were not as clean and not as accurate as those obtained by Li et al.; this surprisingly good result could be

attributed to the correct recovery of $\mu$ and $\gamma$ in spite of a relatively coarse velocity lattice.

The effect of nonreflecting boundary conditions on aeroacoustic simulations was investigated and good results were obtained [19]. Further verification of this modeled BE by considering acoustic scattering of a sinusoidal pulse by a zero circulation vortex and acoustic interaction with a line heat source is also carried out. This way, the ability of the modeled BE to replicate sound scattering and the effect of the Prandtl number on sound propagation could be assessed.

## Conclusions

It has been shown that the complete set of unsteady compressible Navier–Stokes equations can be derived from an improved BGK modeled Boltzmann equation. Thus formulated, the first coefficient of viscosity and the thermal conductivity are recovered correctly, together with the specific heat ratio for diatomic gases.

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